1-Butanol, 2,2,3,3,4,4,4-heptafluoro-

375-01-9 | DTXSID4059914

Model Performance

Model	Data
Model	Dala

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.81	0.55	0.81	0.54	0.71	0.61

Model Results

Predicted value: 570 L/kg

Global applicability domain: Inside

Local applicability domain index: 5.23e-01

Confidence level: 8.19e-01

Nearest Neighbors from the Training Set

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2,4-Dichloroaniline Measured: 525 Predicted: 465 Image not found

Dichlobenil Measured: 316 Predicted: 328 Image not found

2,4-Dichlorophenol Measured: 646 Predicted: 497

Image not found

3,4-Dichlorophenol Measured: 1230 Predicted: 497 Image not found

2,3-Dichlorophenol Measured: 457 Predicted: 577